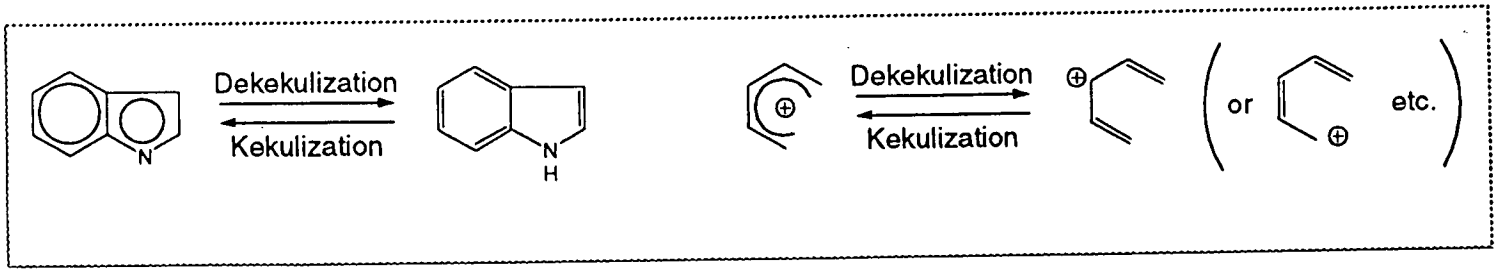

Dekekulization
Kekulization
N
H
Dekekulization
Kekulization
or
etc.

FIG. 1

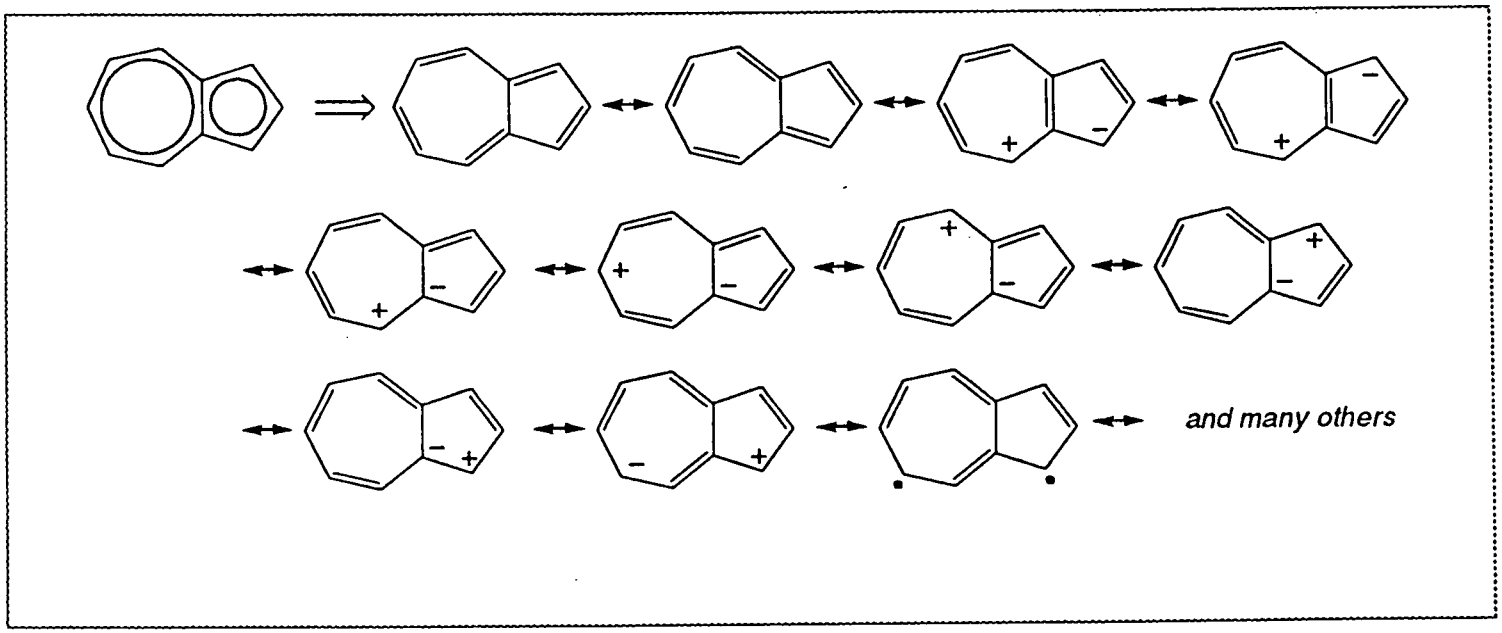


FIG. 2

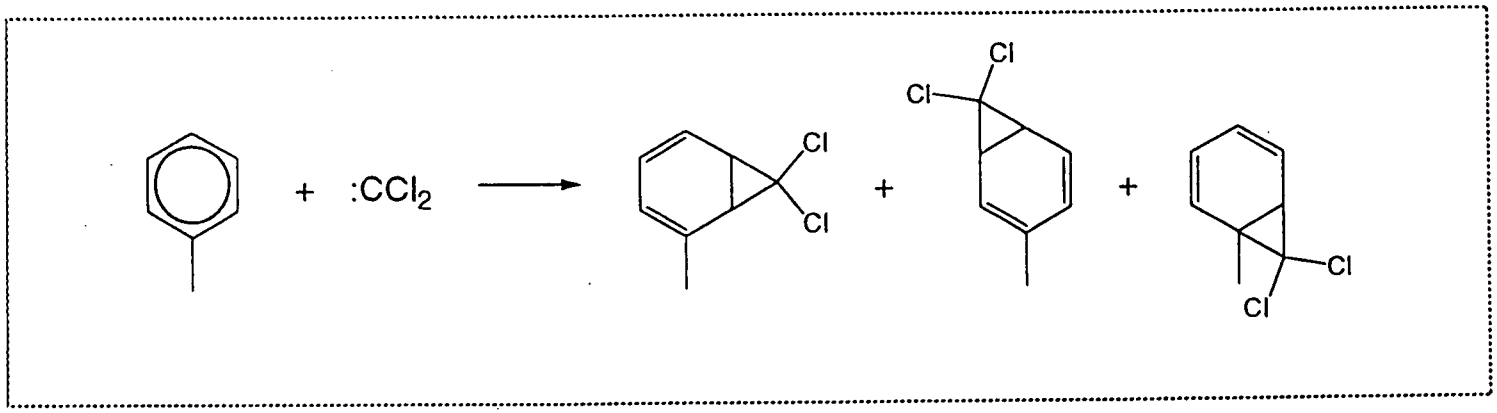


FIG. 3

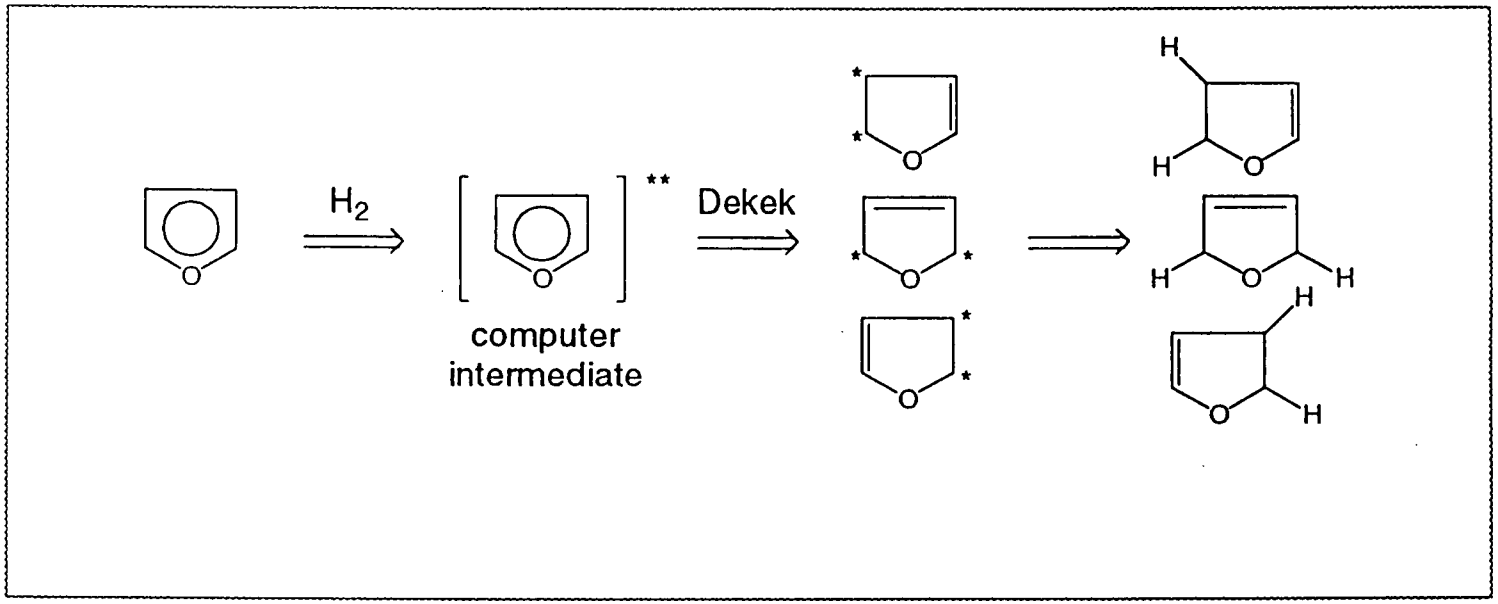


FIG. 4

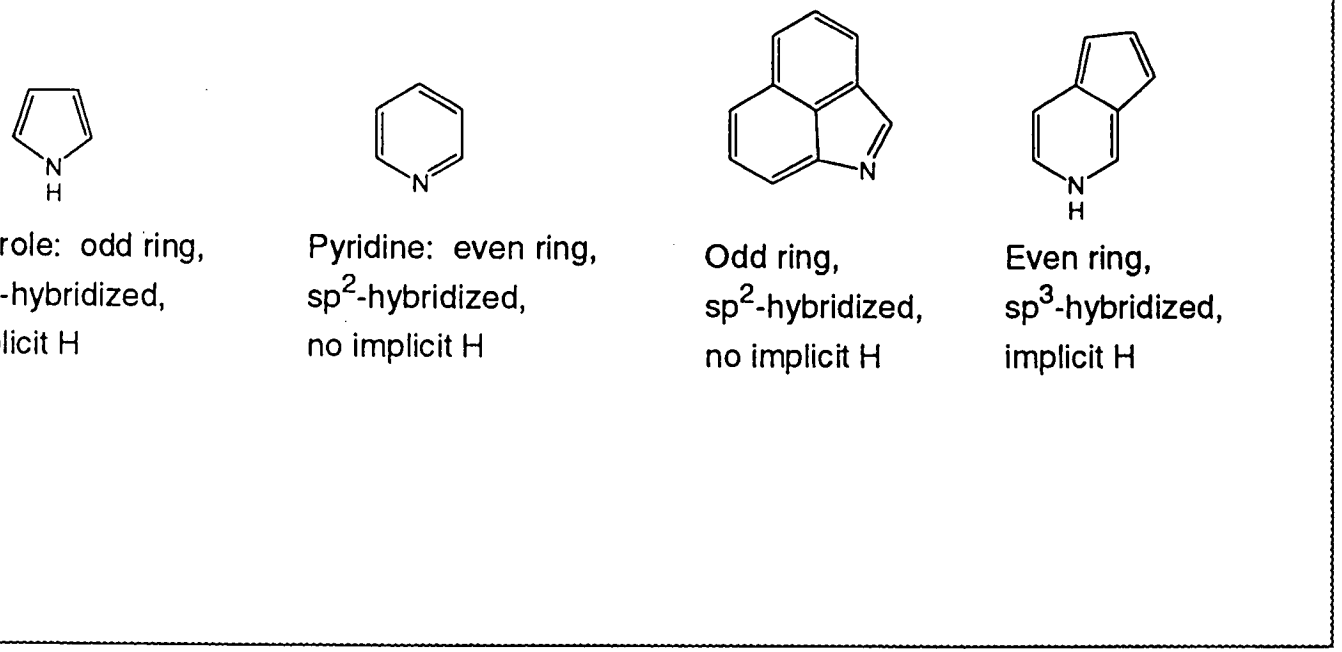

Pyrrole: odd ring, sp3-hybridized, implicit H
Pyridine: even ring, sp2-hybridized, no implicit H
Odd ring, sp2-hybridized, no implicit H
Even ring, sp3-hybridized, implicit H

FIG. 5

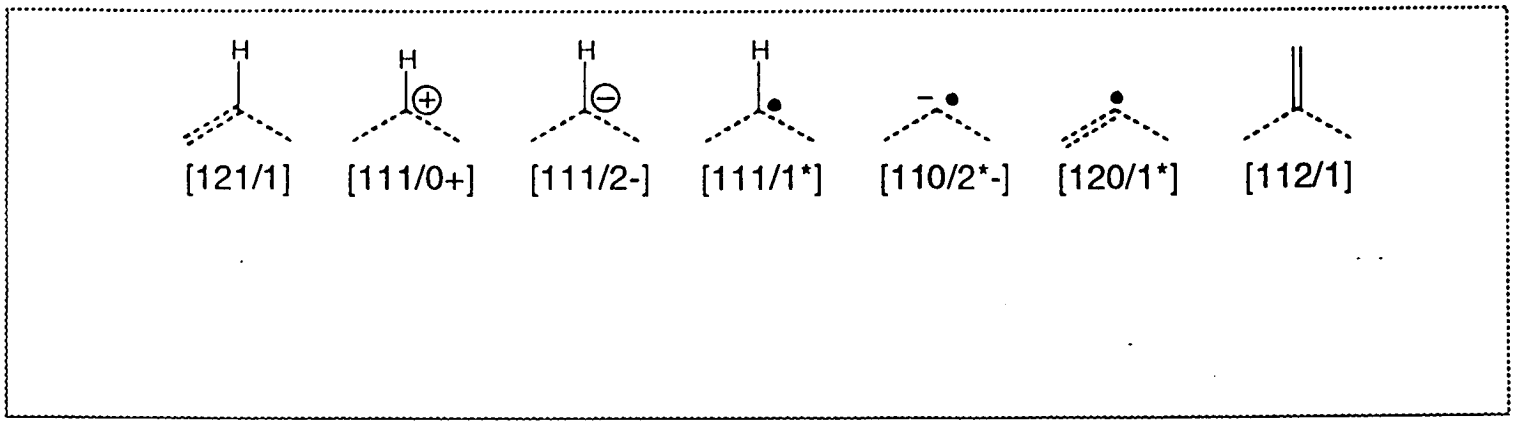


FIG. 6

Table 1. Selected Electronic State/Valence Distributions[a]

Elm	Chrg	Rad	Bd#1	Bd#2	#Extern Bds[b]	#e's Contrib	Shorthand	Structure
B			1	2	0	1	[120/1]	B-1
B			1	1	1	0	[111/0]	B-2
B	-1		1	2	1	1	[121/1-]	B-3
C			1	2	1	1	[121/1]	C-1
C	+1		1	1	1	0	[111/0+]	C-2
C	-1		1	1	1	2	[111/2-]	C-3
C		•	1	1	1	1	[111/1*]	C-4
C			1	1	2	1	[112/1]	C-5
N			1	2	0	1	[120/1]	N-1
N			1	1	1	2	[111/2]	N-2
N	+1		1	2	1	1	[121/1+]	N-3
N	+1	•	1	1	1	1	[111/1+*]	N-4
O			1	1	0	2	[110/2]	O-1
O	+1		1	1	1	2	[111/2+]	O-2
O	+1		1	2	0	1	[120/1+]	O-3
P	like N[c]							
P			1	2	2	1	[122/1]	P-1
S	like O							
S			2	2	0	2	[220/2]	S-1
Cl	+1		1	1	0	2	[110/2+]	Cl-1
Cl			1	2	2	1	[122/1]	Cl-2
Cl			1	2	4	1	[124/1]	Cl-3

FIG. 7

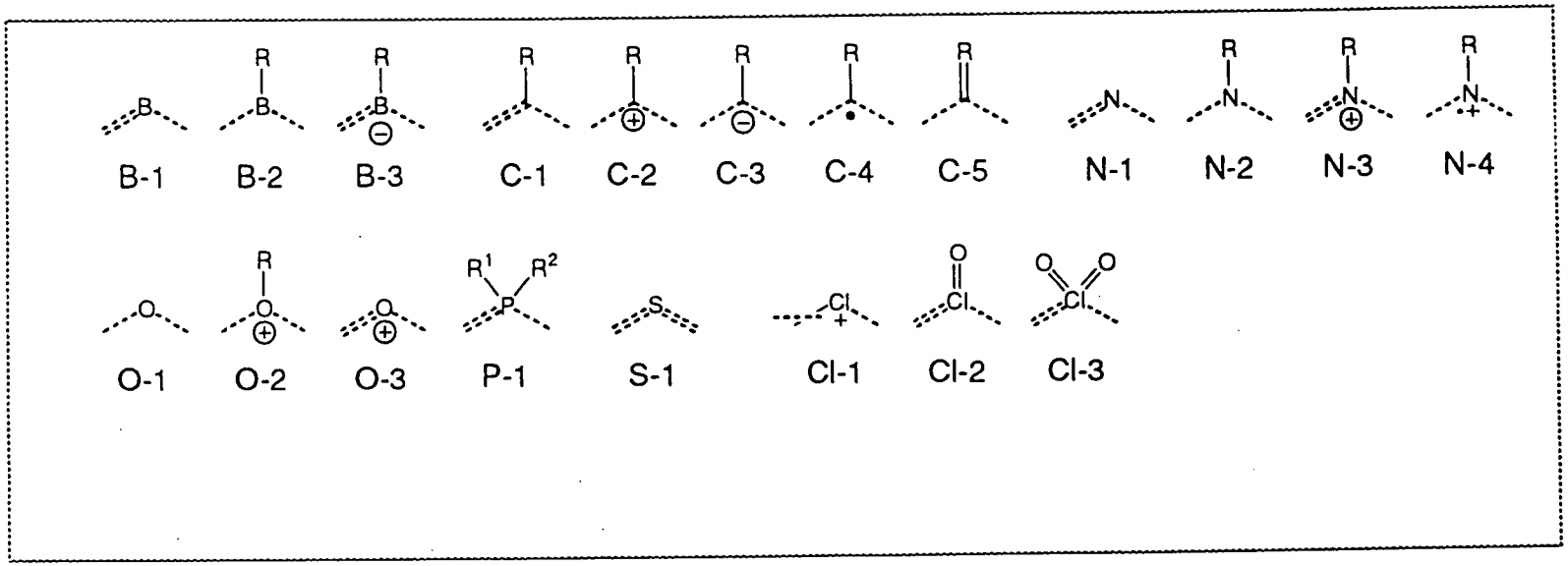


FIG. 8

Table 2. Procedure Control Flags

Flag	Meaning
kDontAssumeImpH	Otherwise, heteroatoms might carry undrawn hydrogens.
kIfFailWithOneSystem_FailWithAll	If given two or more delocalized systems and one fails, the molecule is returned unchanged, and the procedure fails.
kDoNotCreateCharges	Do not create zwitterions, i.e., more charges than necessary to achieve the system's net charge.
kDoNotCreateRadicals	Do not create more than one radical.
kConfineChargesToHeteroatoms	All charged atoms must be heteroatoms.
kConfineRadicalsToHeteroatoms	All atoms with an unpaired electron must be heteroatoms.
kFavorMultiplyBondedHetero	When a system can support more or fewer multiple bonds, favor the form with more multiple bonds (even if it is anti-aromatic).
kDisfavorAntiaromaticSystems	Use this flag in conjunction with the previous.
kSolutionMustBeFullyAlternating	Bonds must alternate as single and double.

FIG. 9

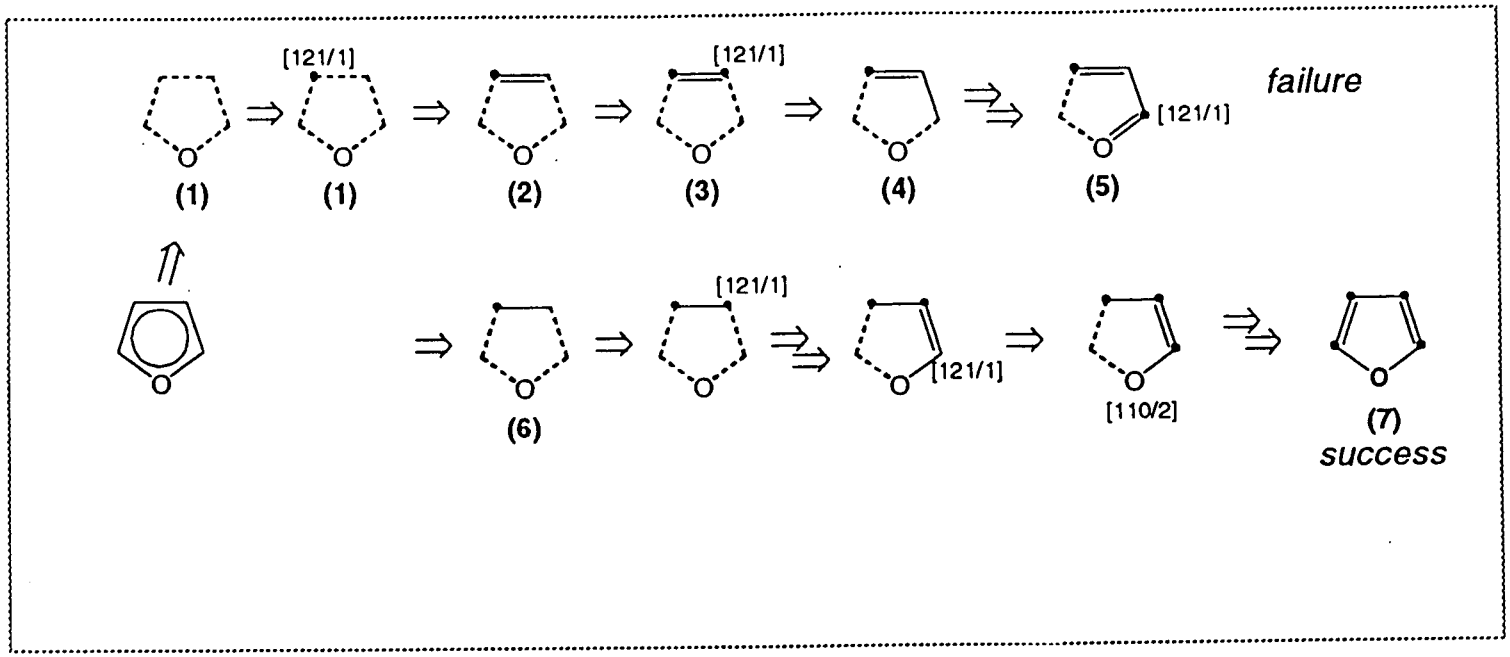
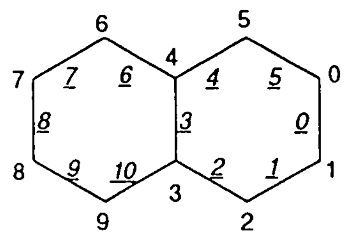


FIG. 10

Table 3. Meanings of bits in the ESVD Screening Bitmask (ESB) and Atom Screening Bitmask (ASB)

Bit #	Description	Bit #	Description
0	Has an internal single bond	8	Charge = 0
1	Has two internal single bonds	9	Charge = +1
2	Has an internal double bond	10	Charge = -1
3	Has two internal double bonds	11	Charge ≠ -1
4	Has an external bond	12	Charge ≠ +1
5	Does *not* have an external bond	13	Radical present
		14	Radical not present

FIG. 11



Atom path = [0,1,2,3,4,5,**0**, 9,8,7,6,**4**]
Bond path = [0,1,2,3,4,5 10,9,8,7,6]

FIG. 12

Action #	Action	Atom / Bond	Action #	Action	Atom or Bond
1	Assign ESVD	Atom 0	14	Assign Bond	Bond 10
2	Assign Bond	Bond 0	15	Assign ESVD	Atom 9
3	Assign ESVD	Atom 1	16	Assign Bond	Bond 9
4	Assign Bond	Bond 1	17	Assign ESVD	Atom 8
5	Assign ESVD	Atom 2	18	Assign Bond	Bond 8
6	Assign Bond	Bond 2	19	Assign ESVD	Atom 7
7	Assign ESVD	Atom 3	20	Assign Bond	Bond 7
8	Assign Bond	Bond 3	21	Assign ESVD	Atom 6
9	Assign ESVD	Atom 4	22	Assign Bond	Bond 6
10	Assign Bond	Bond 4	23	Verify completed	Atom 4
11	Assign ESVD	Atom 5	24	Complete	---
12	Assign Bond	Bond 5			
13	Verify completed	Atom 0			

FIG. 13

Table 4. The Actions Comprising a Strategy

Action	Applies To	Explanation
Assign ESVD	Atom	Find the ESVD's for the current atom that are compatible with its environment. The best one is used directly, and if there is more than one, the rest are queued.
Assign Bond	Bond	Assign a bond order to the current bond, consistent with the ESVD of the previous atom, i.e. the (earliest occurring) atom adjacent to the bond. (The bond's other atom has not been encountered yet, unless the bond closes a ring. Even in this case, the other atom's environment is not taken into account. It will be checked in the next Action.)
Verify Completed	Atom	This Action is taken just after the last bond in a ring or acyclic chain is fixed. Ordinarily the bonds of an atom are sure to be compatible with its assigned ESVD because its ESVD was picked to be compatible with the bond leading to it, and the bond leading away from it was selected to be compatible with its ESVD. However, a ring closure atom has not had its ESVD checked with respect to the ring closure bond, nor has a terminal atom in an acyclic chain. Thus, in this Action the atom is checked to verify that its final bonding environment is compatible with its ESVD.
Complete	---	Signifies that the path is completed, and all atoms have been assigned compatible ESVD's and bond orders. If the net charge or radical count of the putative solution is wrong, the solution is rejected. If the solution is perfect, as defined elsewhere, it is returned directly and the procedure terminates. Otherwise, if it is the best solution yet, it displaces the previous best candidate.

FIG. 14

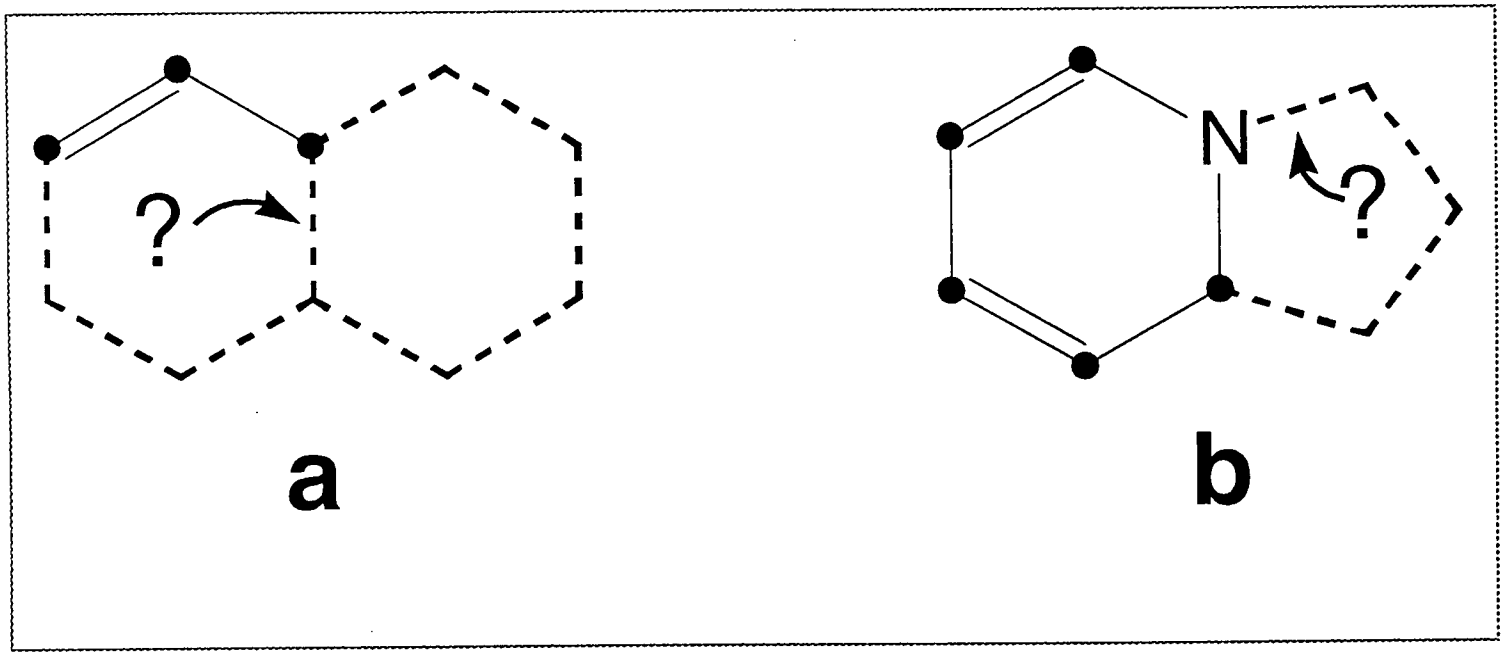
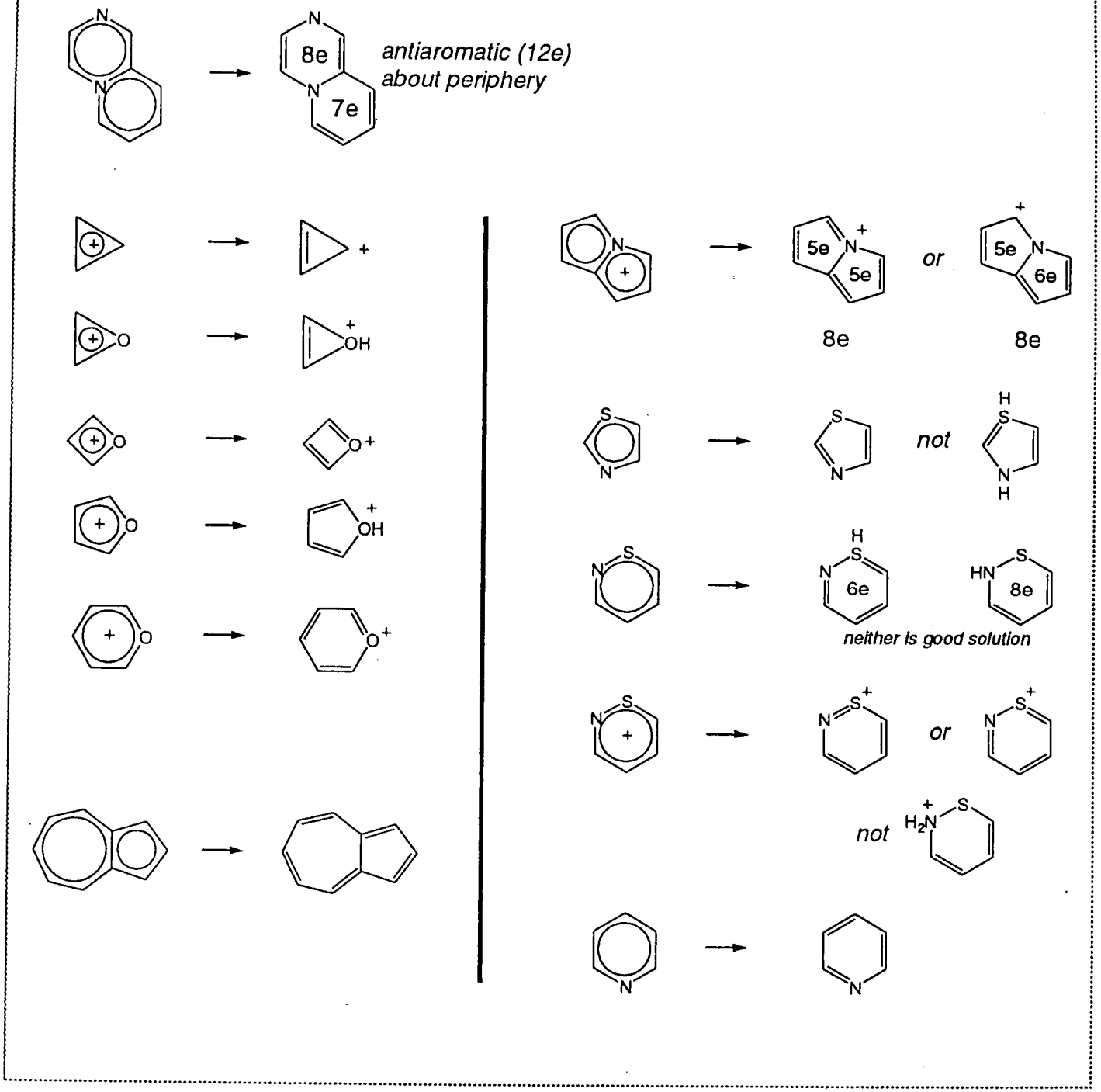


FIG. 15

FIG. 16


8e
7e
antiaromatic (12e)
about periphery
5e
5e
or
5e
6e
8e
8e
not
6e
8e
neither is good solution
or
not

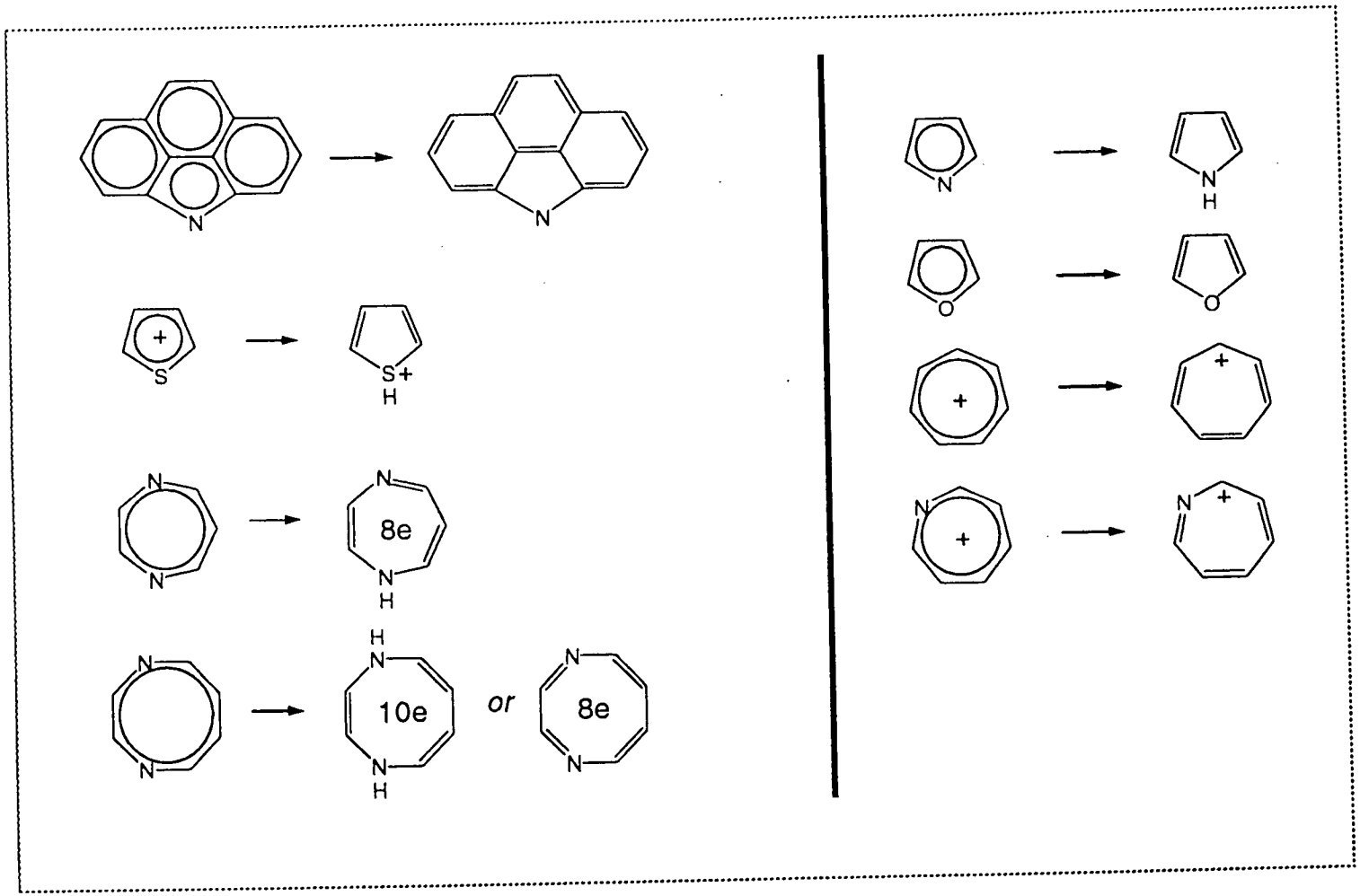


FIG. 17

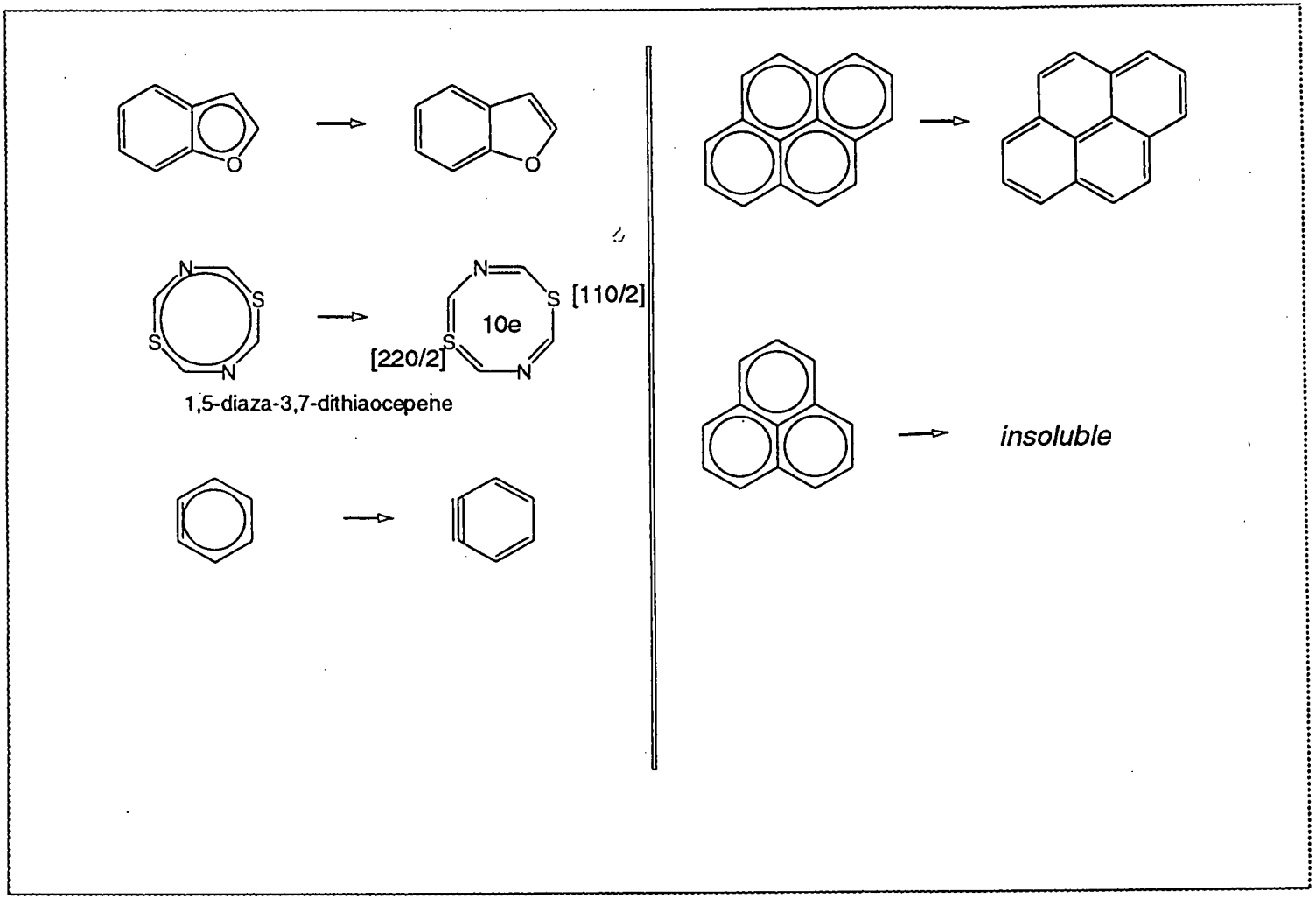


FIG. 18

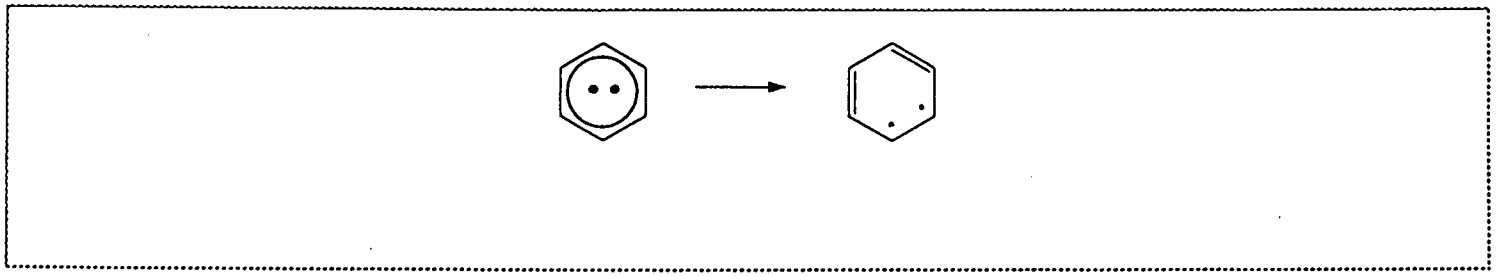


FIG. 19

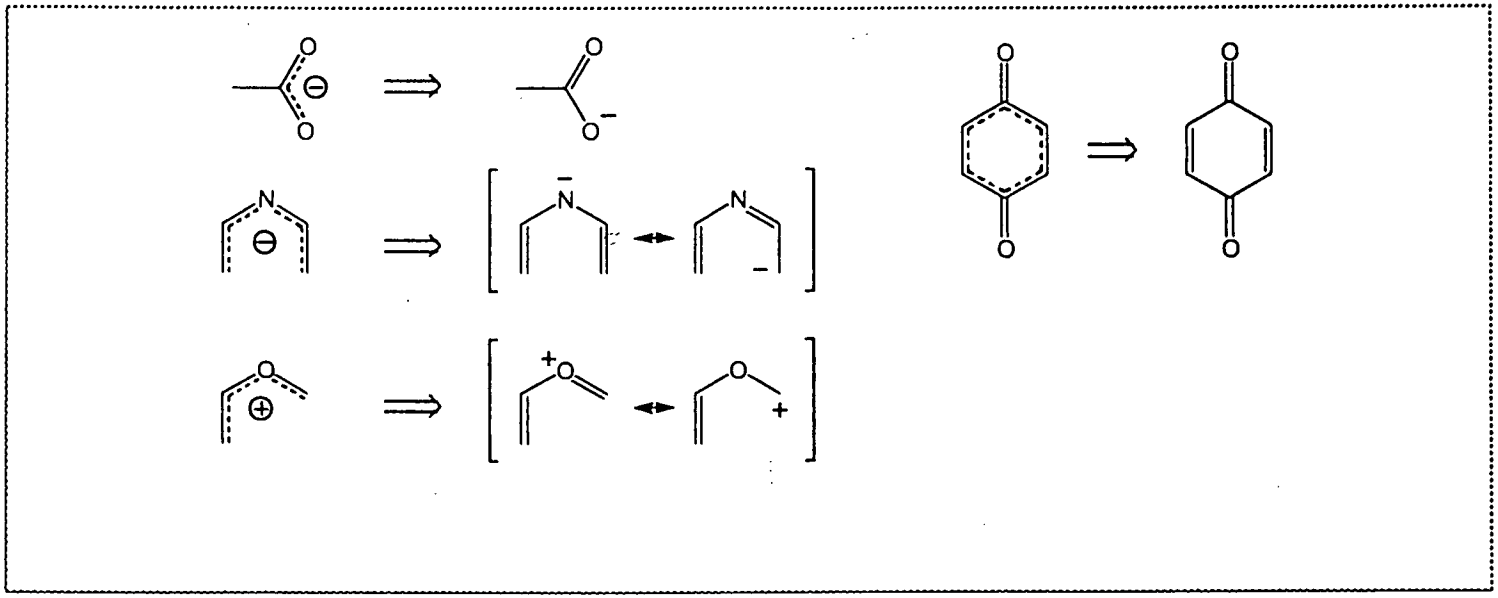


FIG. 20

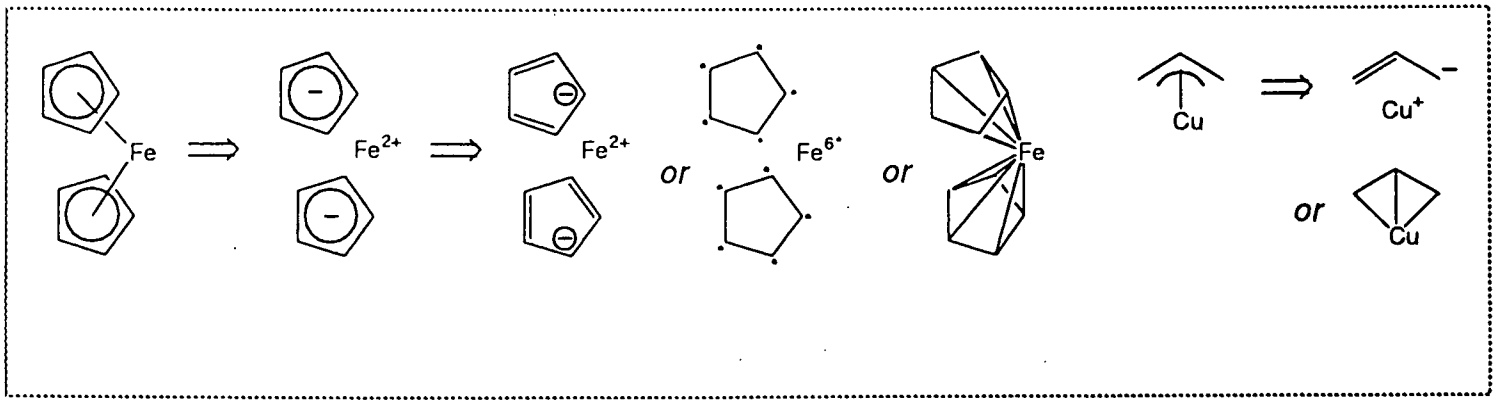


FIG. 21

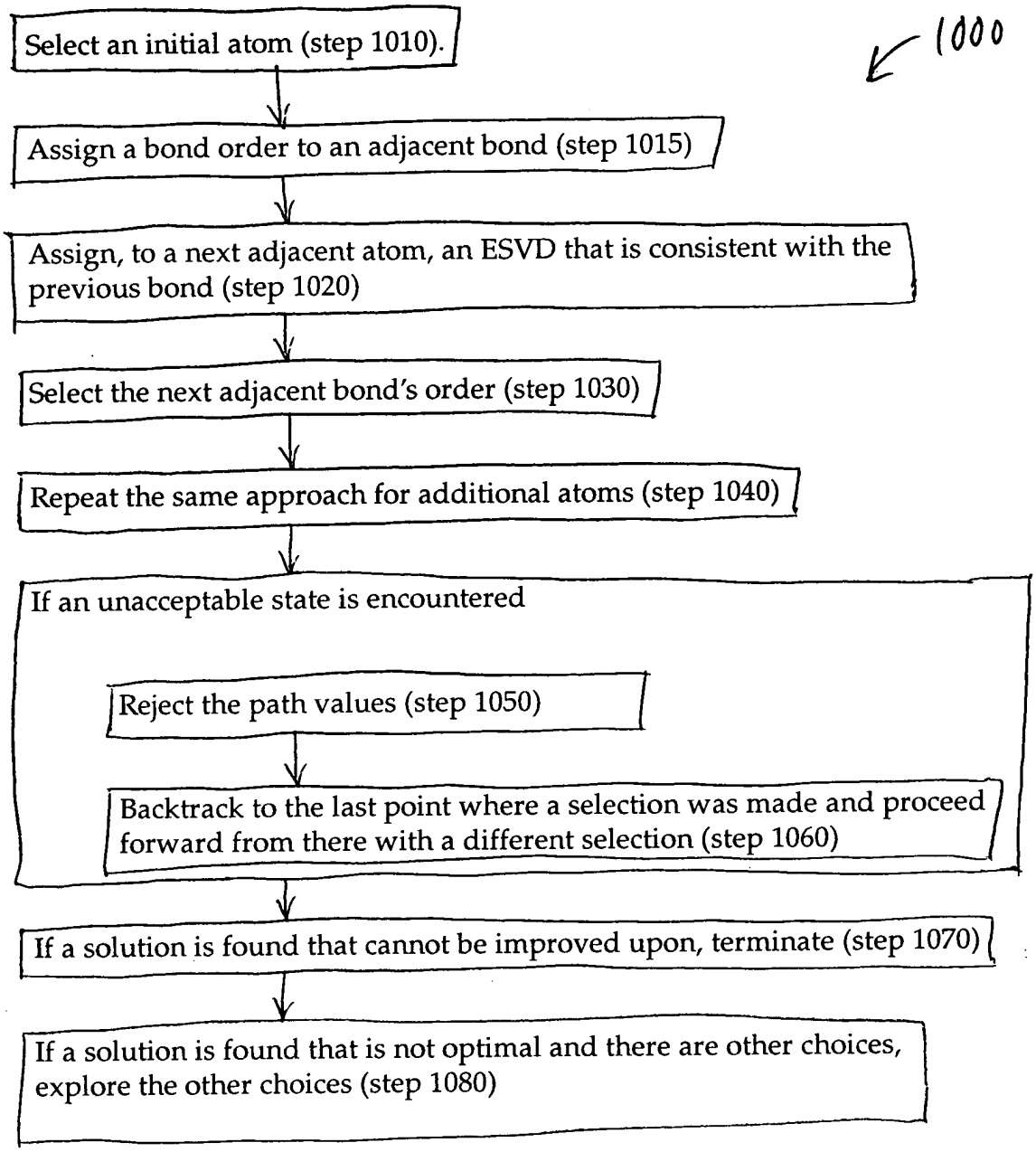

1000
Select an initial atom (step 1010).
Assign a bond order to an adjacent bond (step 1015)
Assign, to a next adjacent atom, an ESVD that is consistent with the previous bond (step 1020)
Select the next adjacent bond's order (step 1030)
Repeat the same approach for additional atoms (step 1040)
If an unacceptable state is encountered
Reject the path values (step 1050)
Backtrack to the last point where a selection was made and proceed forward from there with a different selection (step 1060)
If a solution is found that cannot be improved upon, terminate (step 1070)
If a solution is found that is not optimal and there are other choices, explore the other choices (step 1080)

FIG. 22

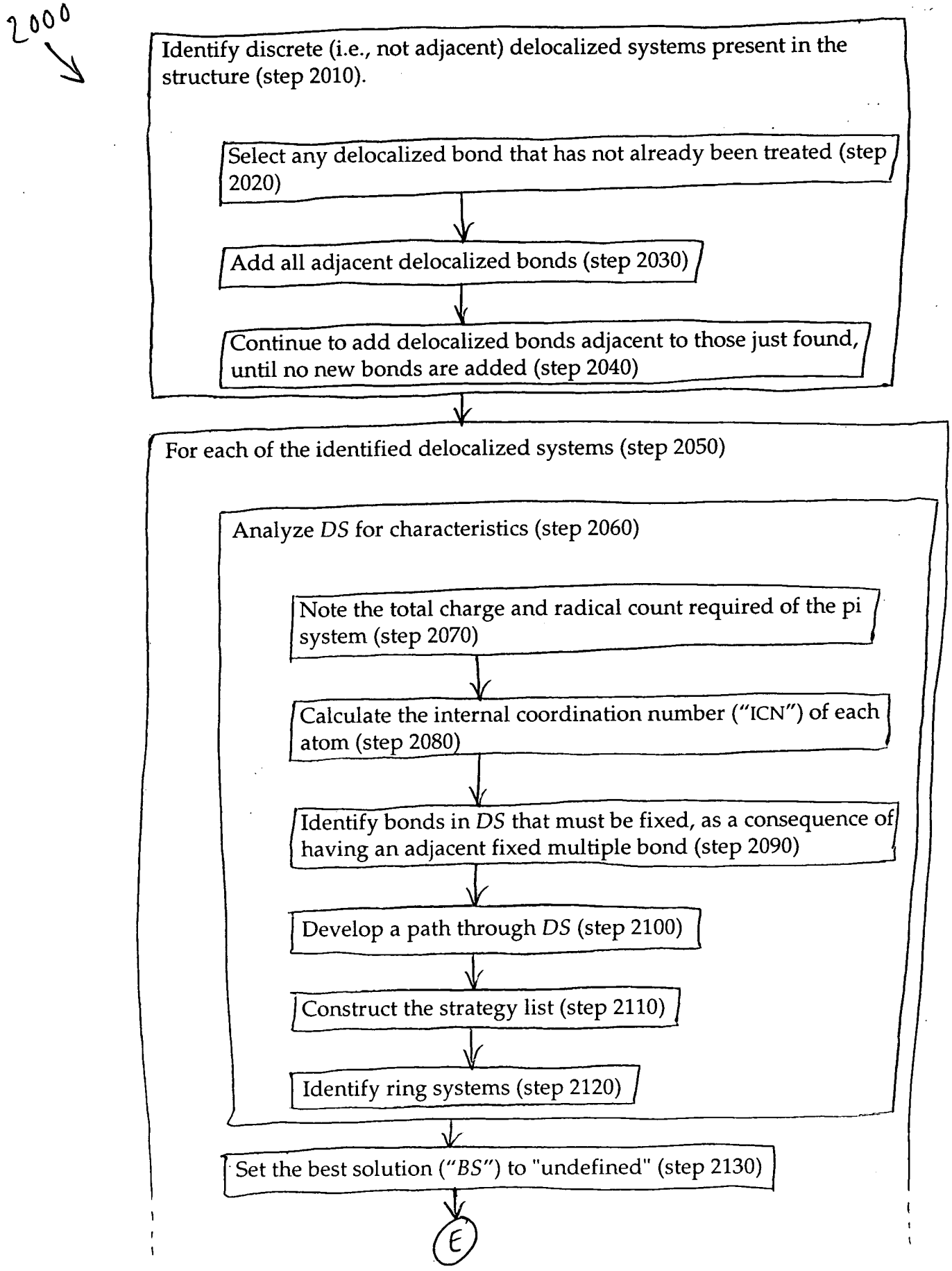

2000
Identify discrete (i.e., not adjacent) delocalized systems present in the structure (step 2010).
Select any delocalized bond that has not already been treated (step 2020)
Add all adjacent delocalized bonds (step 2030)
Continue to add delocalized bonds adjacent to those just found, until no new bonds are added (step 2040)
For each of the identified delocalized systems (step 2050)
Analyze DS for characteristics (step 2060)
Note the total charge and radical count required of the pi system (step 2070)
Calculate the internal coordination number ("ICN") of each atom (step 2080)
Identify bonds in DS that must be fixed, as a consequence of having an adjacent fixed multiple bond (step 2090)
Develop a path through DS (step 2100)
Construct the strategy list (step 2110)
Identify ring systems (step 2120)
Set the best solution ("BS") to "undefined" (step 2130)
E

FIG. 23A

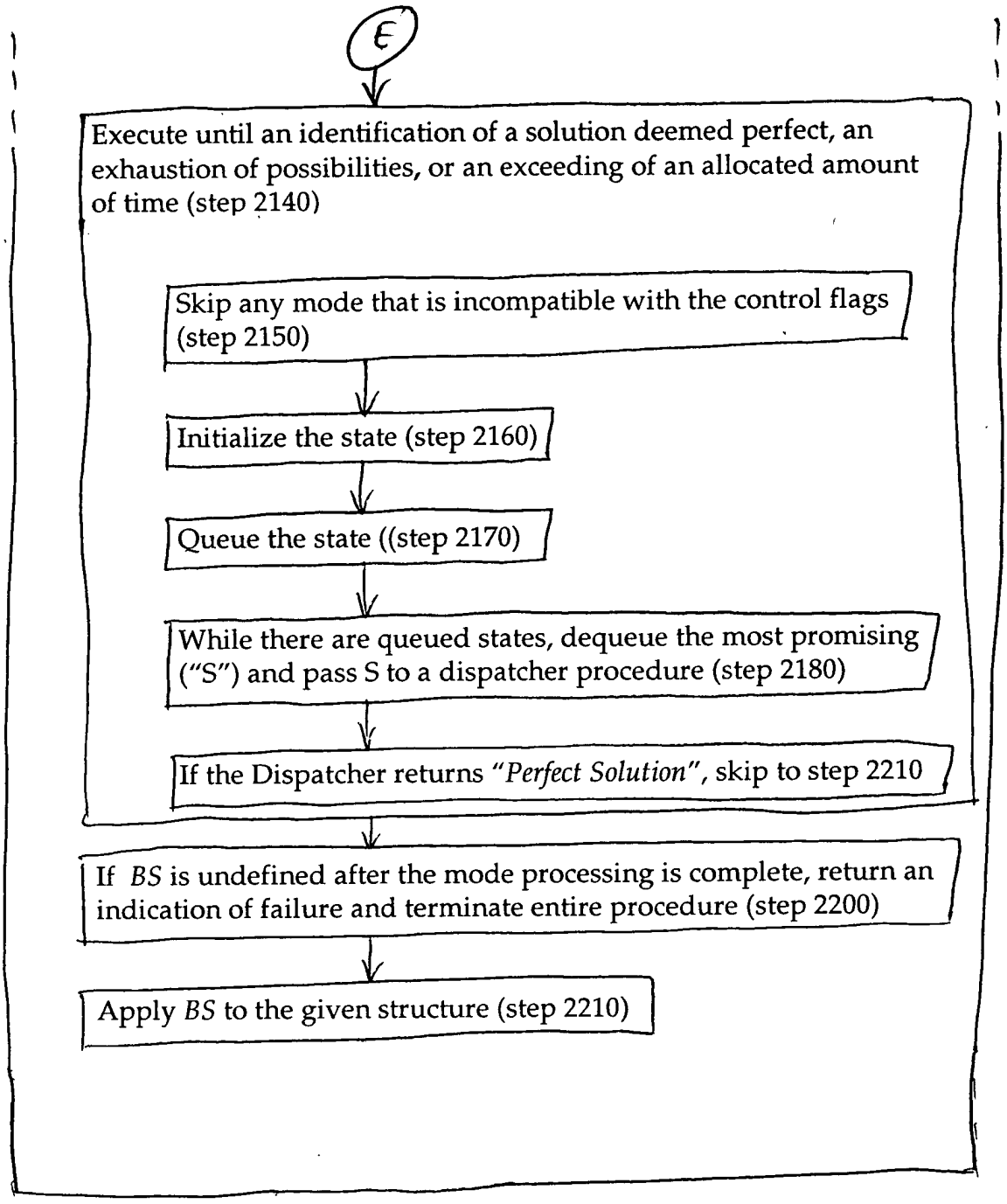

E
Execute until an identification of a solution deemed perfect, an exhaustion of possibilities, or an exceeding of an allocated amount of time (step 2140)
Skip any mode that is incompatible with the control flags (step 2150)
Initialize the state (step 2160)
Queue the state ((step 2170)
While there are queued states, dequeue the most promising ("S") and pass S to a dispatcher procedure (step 2180)
If the Dispatcher returns "Perfect Solution", skip to step 2210
If BS is undefined after the mode processing is complete, return an indication of failure and terminate entire procedure (step 2200)
Apply BS to the given structure (step 2210)

FIG. 23B

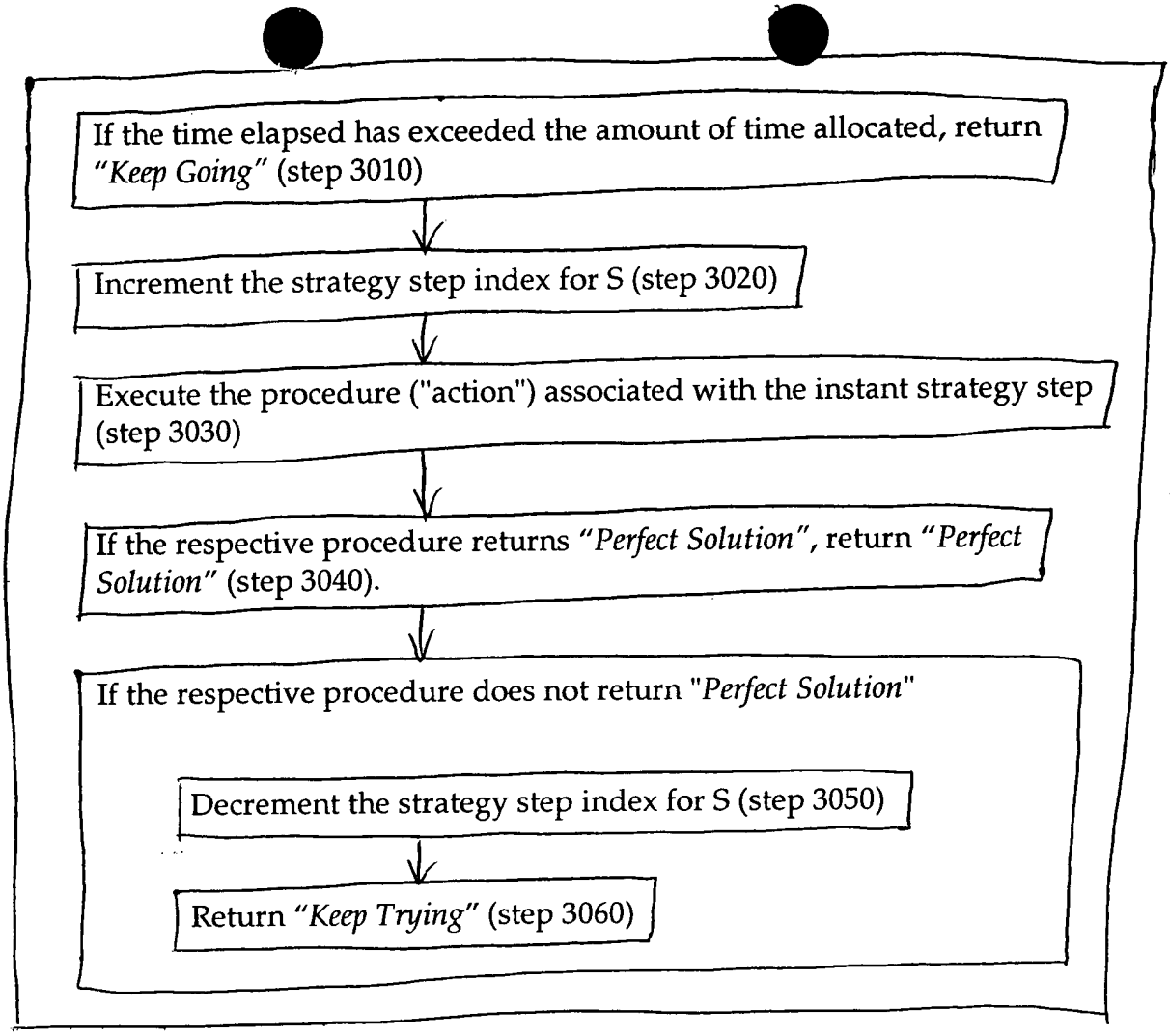

3000
If the time elapsed has exceeded the amount of time allocated, return "Keep Going" (step 3010)
Increment the strategy step index for S (step 3020)
Execute the procedure ("action") associated with the instant strategy step (step 3030)
If the respective procedure returns "Perfect Solution", return "Perfect Solution" (step 3040).
If the respective procedure does not return "Perfect Solution"
Decrement the strategy step index for S (step 3050)
Return "Keep Trying" (step 3060)

FIG. 24

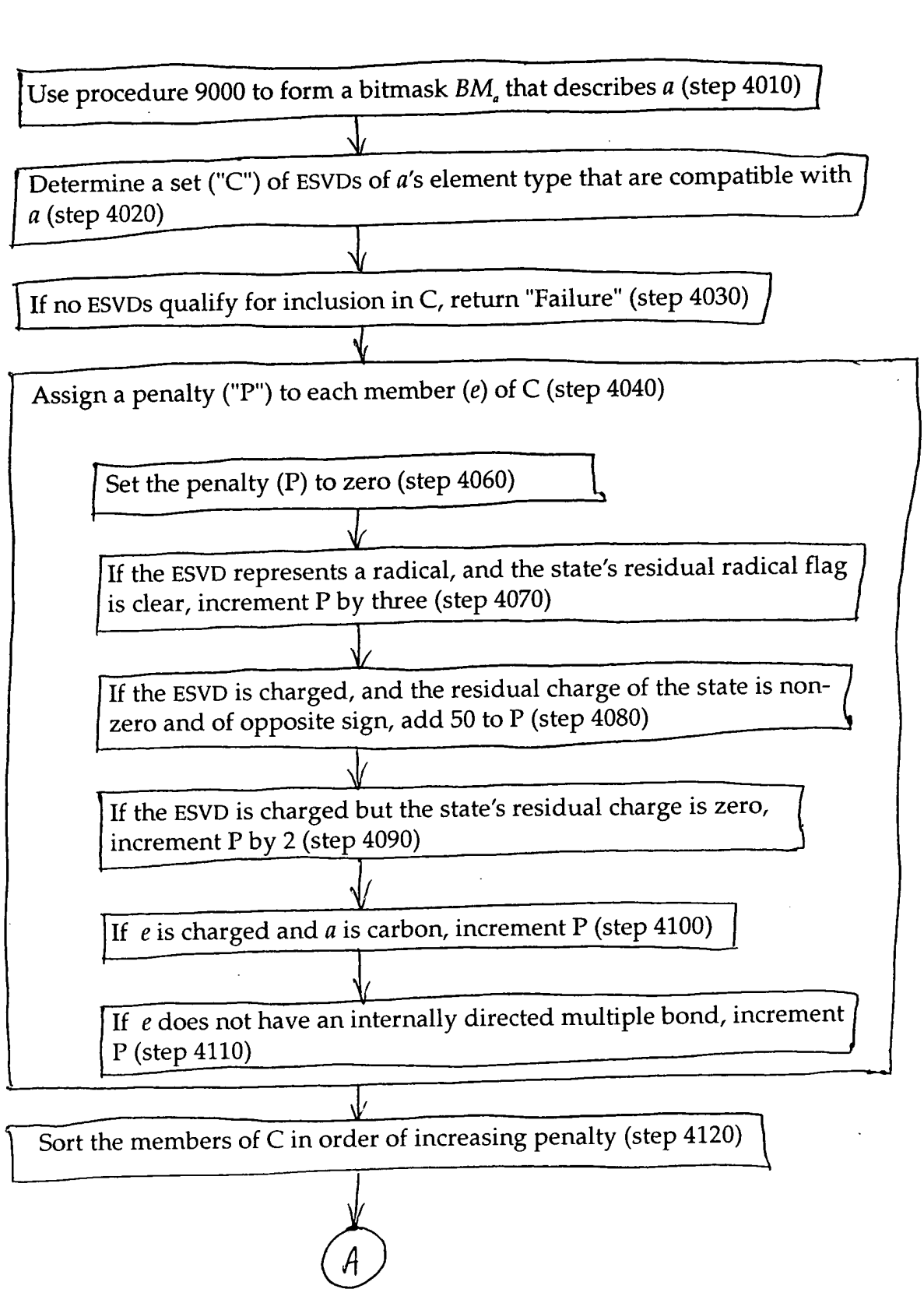

4000
Use procedure 9000 to form a bitmask BM_a that describes a (step 4010)
Determine a set ("C") of ESVDs of a's element type that are compatible with a (step 4020)
If no ESVDs qualify for inclusion in C, return "Failure" (step 4030)
Assign a penalty ("P") to each member (e) of C (step 4040)
Set the penalty (P) to zero (step 4060)
If the ESVD represents a radical, and the state's residual radical flag is clear, increment P by three (step 4070)
If the ESVD is charged, and the residual charge of the state is non-zero and of opposite sign, add 50 to P (step 4080)
If the ESVD is charged but the state's residual charge is zero, increment P by 2 (step 4090)
If e is charged and a is carbon, increment P (step 4100)
If e does not have an internally directed multiple bond, increment P (step 4110)
Sort the members of C in order of increasing penalty (step 4120)
A

FIG. 25A

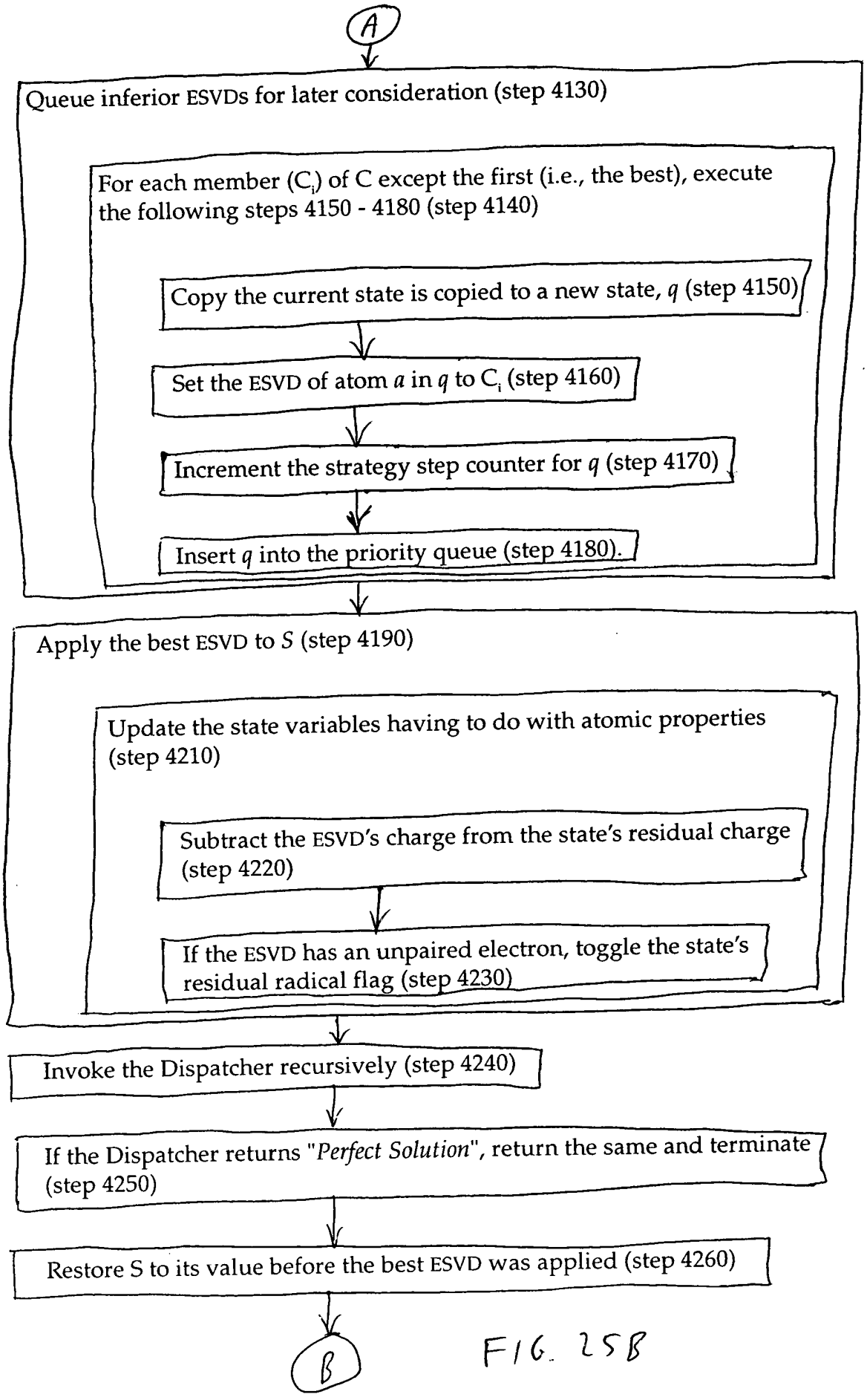

A
Queue inferior ESVDs for later consideration (step 4130)
For each member (C_i) of C except the first (i.e., the best), execute the following steps 4150 - 4180 (step 4140)
Copy the current state is copied to a new state, *q* (step 4150)
Set the ESVD of atom *a* in *q* to C_i (step 4160)
Increment the strategy step counter for *q* (step 4170)
Insert *q* into the priority queue (step 4180).
Apply the best ESVD to *S* (step 4190)
Update the state variables having to do with atomic properties (step 4210)
Subtract the ESVD's charge from the state's residual charge (step 4220)
If the ESVD has an unpaired electron, toggle the state's residual radical flag (step 4230)
Invoke the Dispatcher recursively (step 4240)
If the Dispatcher returns "*Perfect Solution*", return the same and terminate (step 4250)
Restore S to its value before the best ESVD was applied (step 4260)
B

FIG. 25B

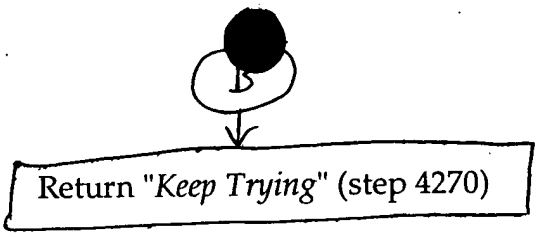


FIG. 25C

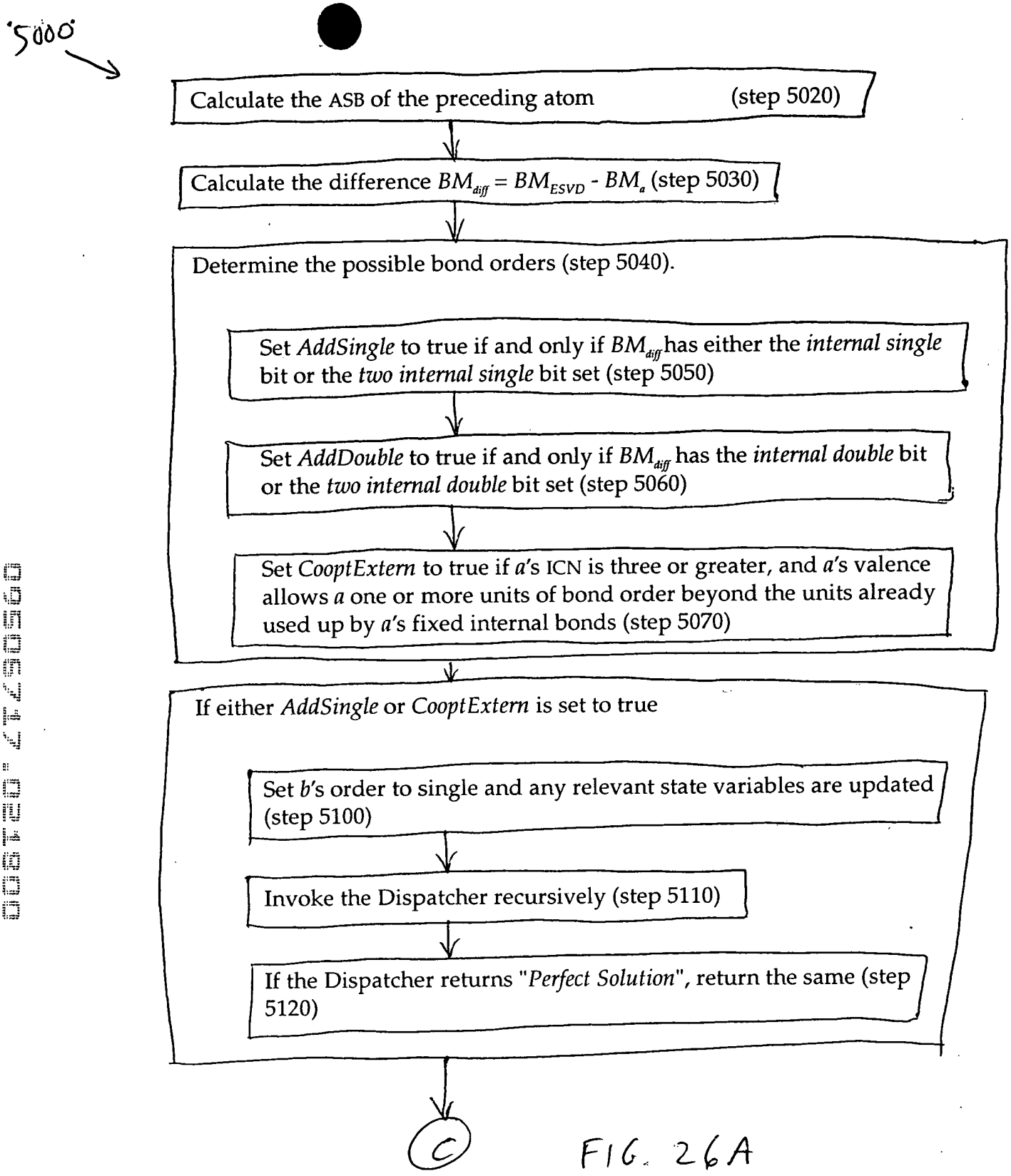

5000
Calculate the ASB of the preceding atom (step 5020)
Calculate the difference $BM_{diff} = BM_{ESVD} - BM_a$ (step 5030)
Determine the possible bond orders (step 5040).
Set *AddSingle* to true if and only if BM_{diff} has either the *internal single* bit or the *two internal single* bit set (step 5050)
Set *AddDouble* to true if and only if BM_{diff} has the *internal double* bit or the *two internal double* bit set (step 5060)
Set *CooptExtern* to true if *a*'s ICN is three or greater, and *a*'s valence allows *a* one or more units of bond order beyond the units already used up by *a*'s fixed internal bonds (step 5070)
If either *AddSingle* or *CooptExtern* is set to true
Set *b*'s order to single and any relevant state variables are updated (step 5100)
Invoke the Dispatcher recursively (step 5110)
If the Dispatcher returns "*Perfect Solution*", return the same (step 5120)
C

FIG. 26A

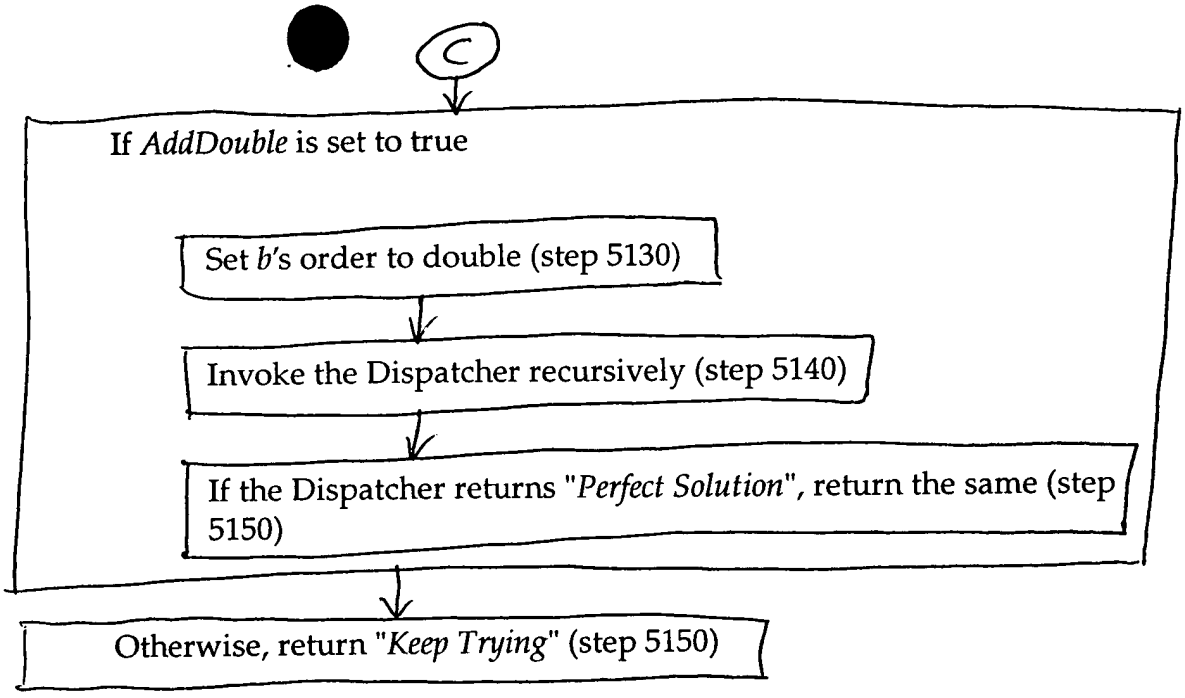

C
If *AddDouble* is set to true
Set *b*'s order to double (step 5130)
Invoke the Dispatcher recursively (step 5140)
If the Dispatcher returns "*Perfect Solution*", return the same (step 5150)
Otherwise, return "*Keep Trying*" (step 5150)

FIG. 26B

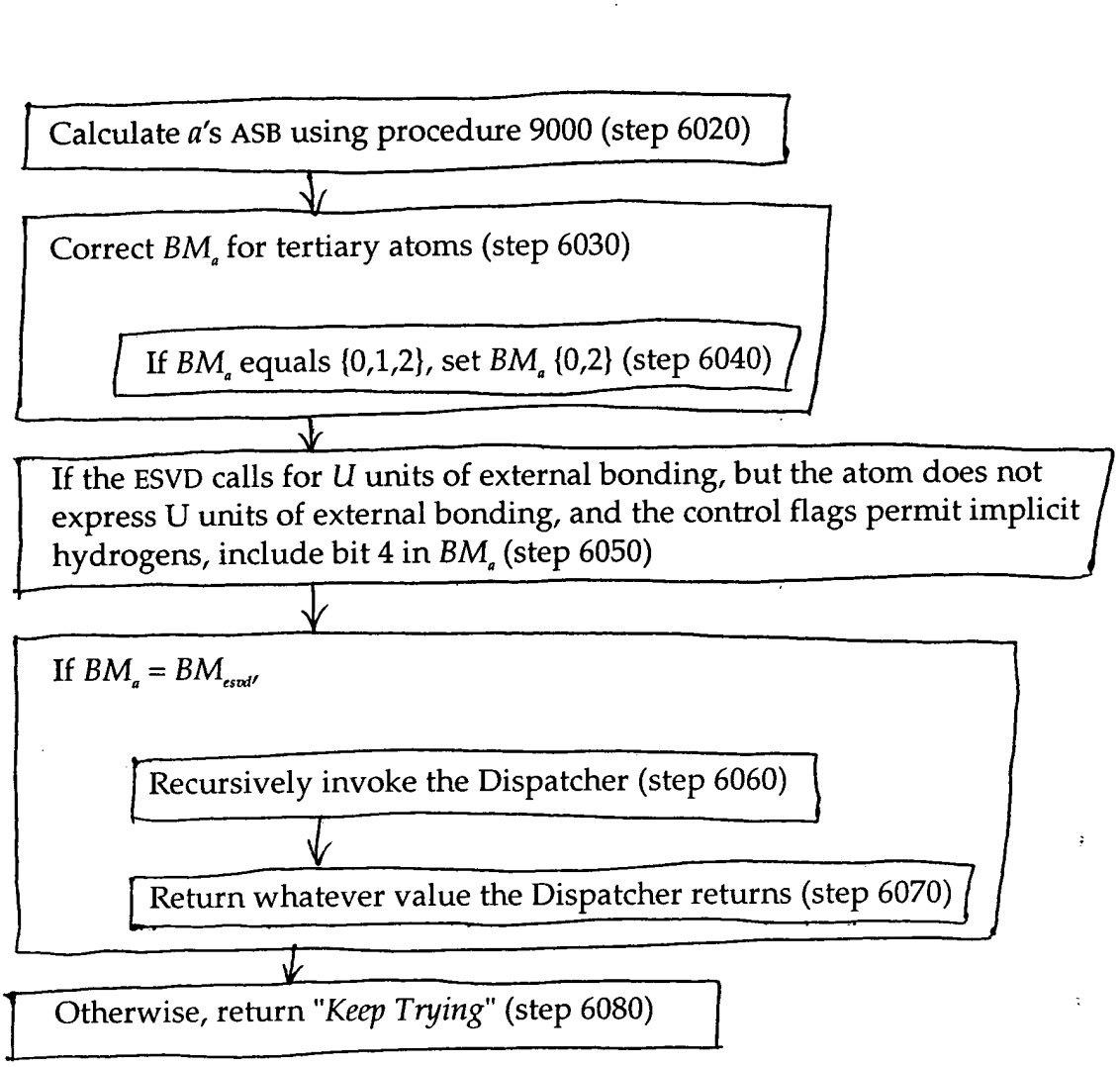

6000
Calculate a's ASB using procedure 9000 (step 6020)
Correct BM_a for tertiary atoms (step 6030)
If BM_a equals {0,1,2}, set BM_a {0,2} (step 6040)
If the ESVD calls for U units of external bonding, but the atom does not express U units of external bonding, and the control flags permit implicit hydrogens, include bit 4 in BM_a (step 6050)
If $BM_a = BM_{esvd'}$
Recursively invoke the Dispatcher (step 6060)
Return whatever value the Dispatcher returns (step 6070)
Otherwise, return "Keep Trying" (step 6080)

FIG 27

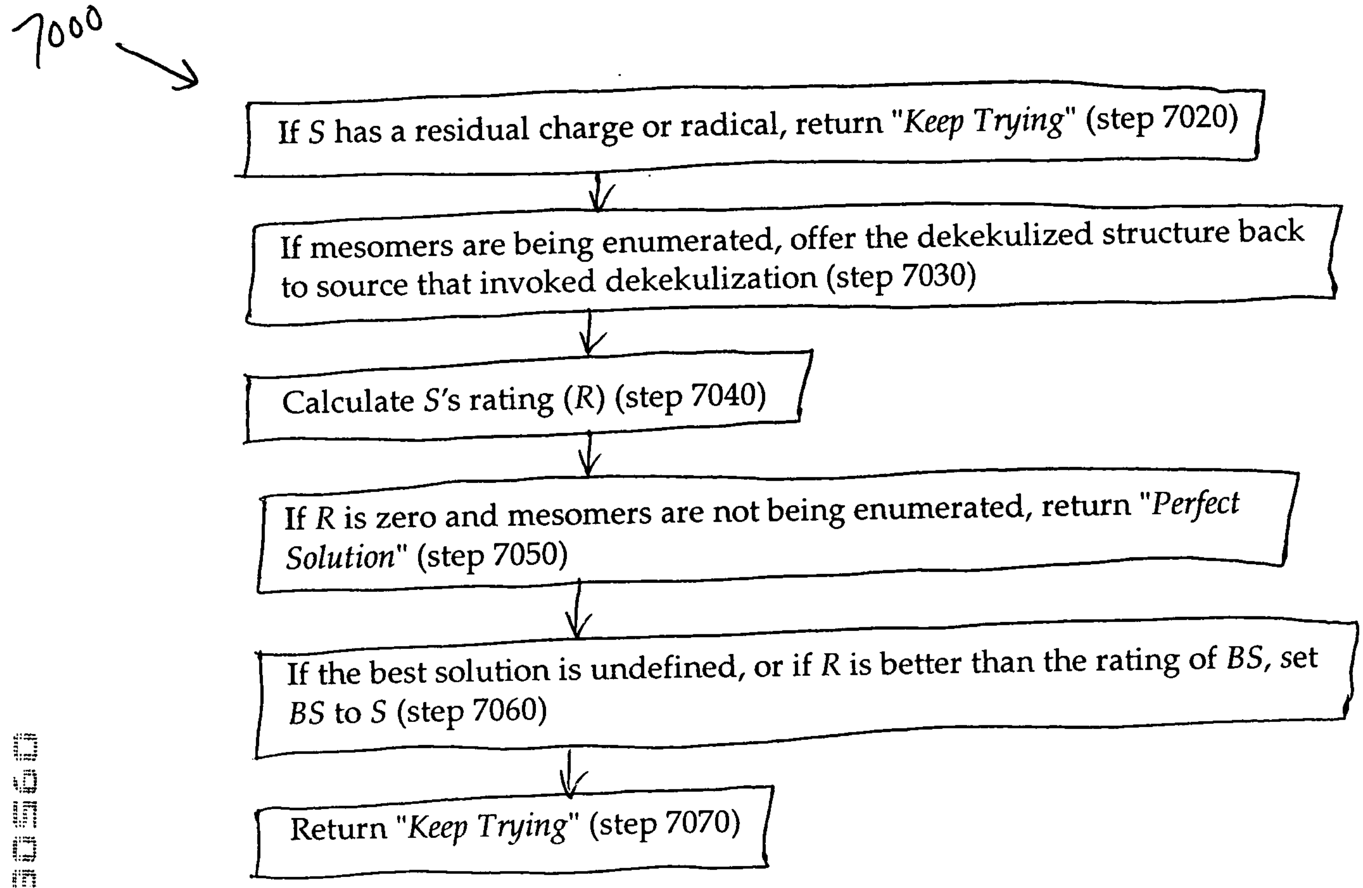

7000
If S has a residual charge or radical, return "Keep Trying" (step 7020)
If mesomers are being enumerated, offer the dekekulized structure back to source that invoked dekekulization (step 7030)
Calculate S's rating (R) (step 7040)
If R is zero and mesomers are not being enumerated, return "Perfect Solution" (step 7050)
If the best solution is undefined, or if R is better than the rating of BS, set BS to S (step 7060)
Return "Keep Trying" (step 7070)

FIG. 28

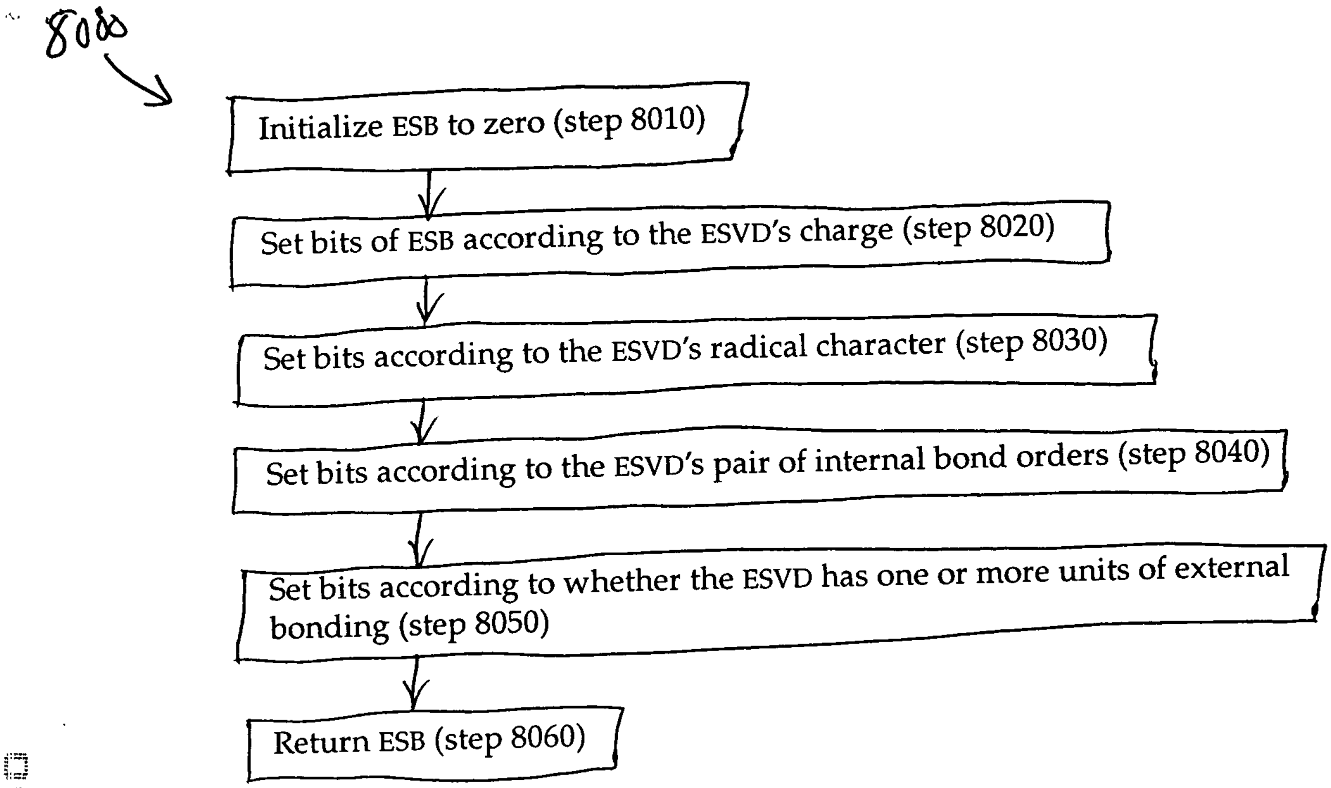

8000
Initialize ESB to zero (step 8010)
Set bits of ESB according to the ESVD's charge (step 8020)
Set bits according to the ESVD's radical character (step 8030)
Set bits according to the ESVD's pair of internal bond orders (step 8040)
Set bits according to whether the ESVD has one or more units of external bonding (step 8050)
Return ESB (step 8060)

FIG. 29

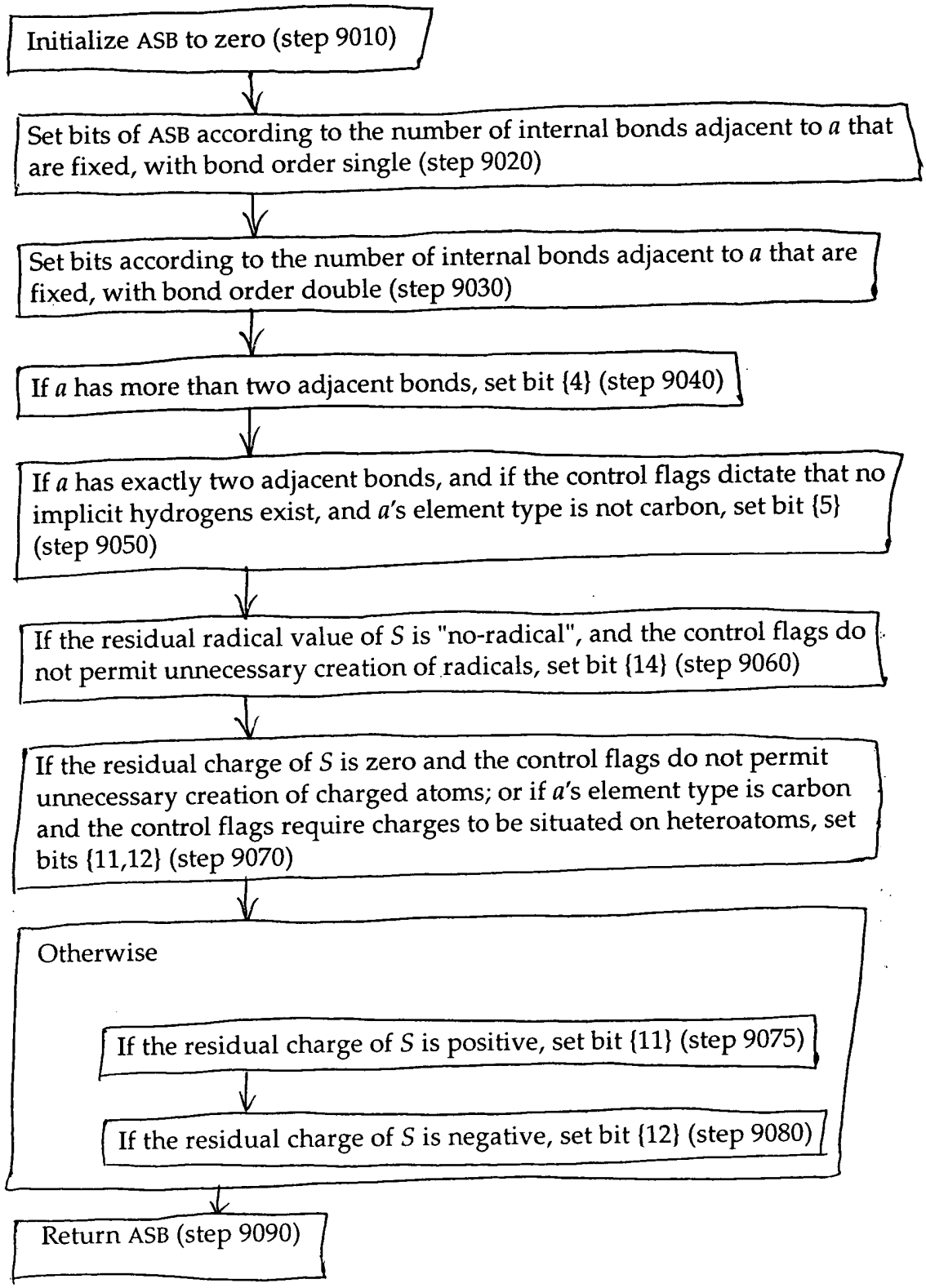

9000
Initialize ASB to zero (step 9010)
Set bits of ASB according to the number of internal bonds adjacent to a that are fixed, with bond order single (step 9020)
Set bits according to the number of internal bonds adjacent to a that are fixed, with bond order double (step 9030)
If a has more than two adjacent bonds, set bit {4} (step 9040)
If a has exactly two adjacent bonds, and if the control flags dictate that no implicit hydrogens exist, and a's element type is not carbon, set bit {5} (step 9050)
If the residual radical value of S is "no-radical", and the control flags do not permit unnecessary creation of radicals, set bit {14} (step 9060)
If the residual charge of S is zero and the control flags do not permit unnecessary creation of charged atoms; or if a's element type is carbon and the control flags require charges to be situated on heteroatoms, set bits {11,12} (step 9070)
Otherwise
If the residual charge of S is positive, set bit {11} (step 9075)
If the residual charge of S is negative, set bit {12} (step 9080)
Return ASB (step 9090)

FIG. 30

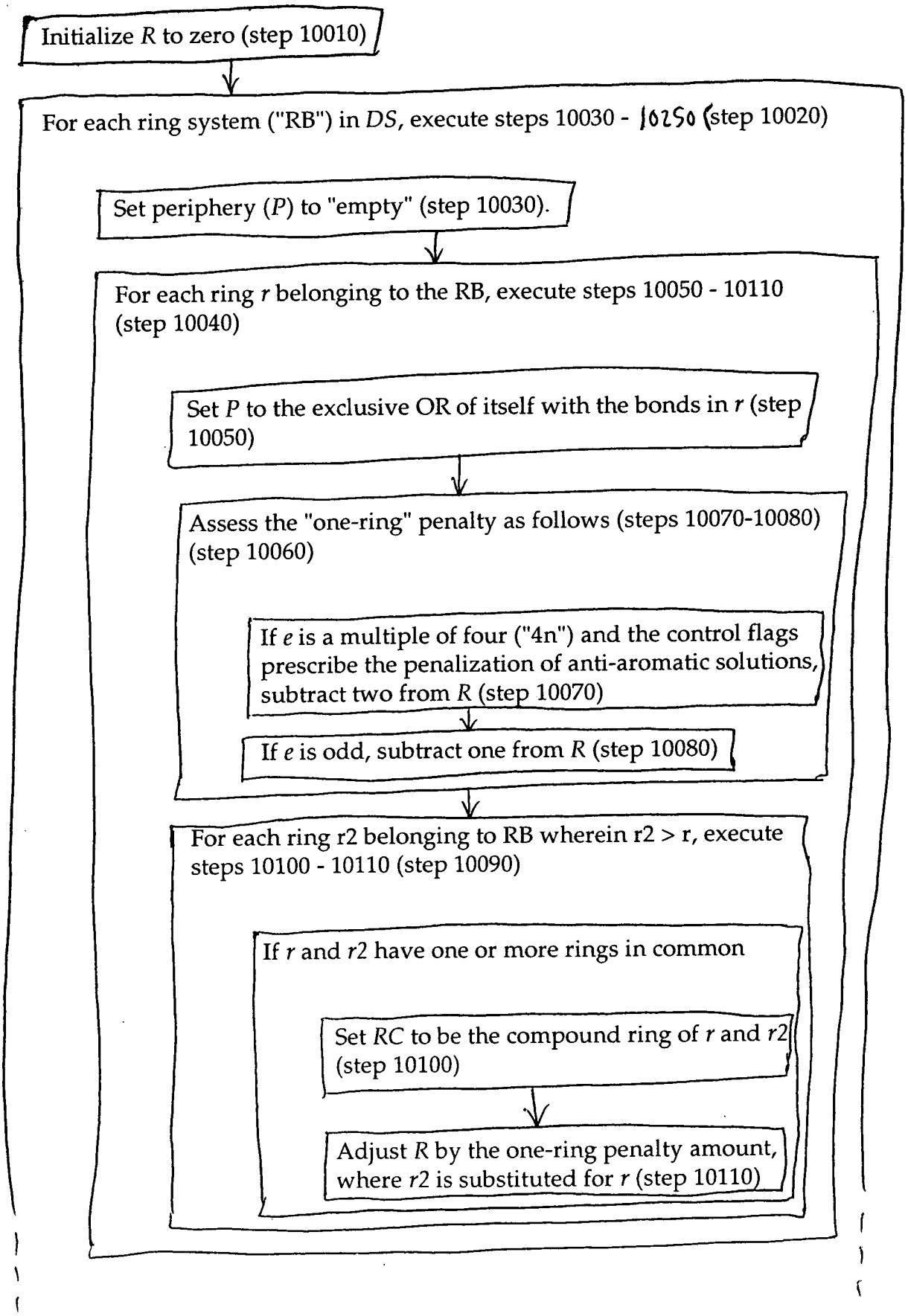

10000
Initialize R to zero (step 10010)
For each ring system ("RB") in DS, execute steps 10030 - 10250 (step 10020)
Set periphery (P) to "empty" (step 10030).
For each ring r belonging to the RB, execute steps 10050 - 10110 (step 10040)
Set P to the exclusive OR of itself with the bonds in r (step 10050)
Assess the "one-ring" penalty as follows (steps 10070-10080) (step 10060)
If e is a multiple of four ("4n") and the control flags prescribe the penalization of anti-aromatic solutions, subtract two from R (step 10070)
If e is odd, subtract one from R (step 10080)
For each ring r2 belonging to RB wherein r2 > r, execute steps 10100 - 10110 (step 10090)
If r and r2 have one or more rings in common
Set RC to be the compound ring of r and r2 (step 10100)
Adjust R by the one-ring penalty amount, where r2 is substituted for r (step 10110)

FIG. 31A

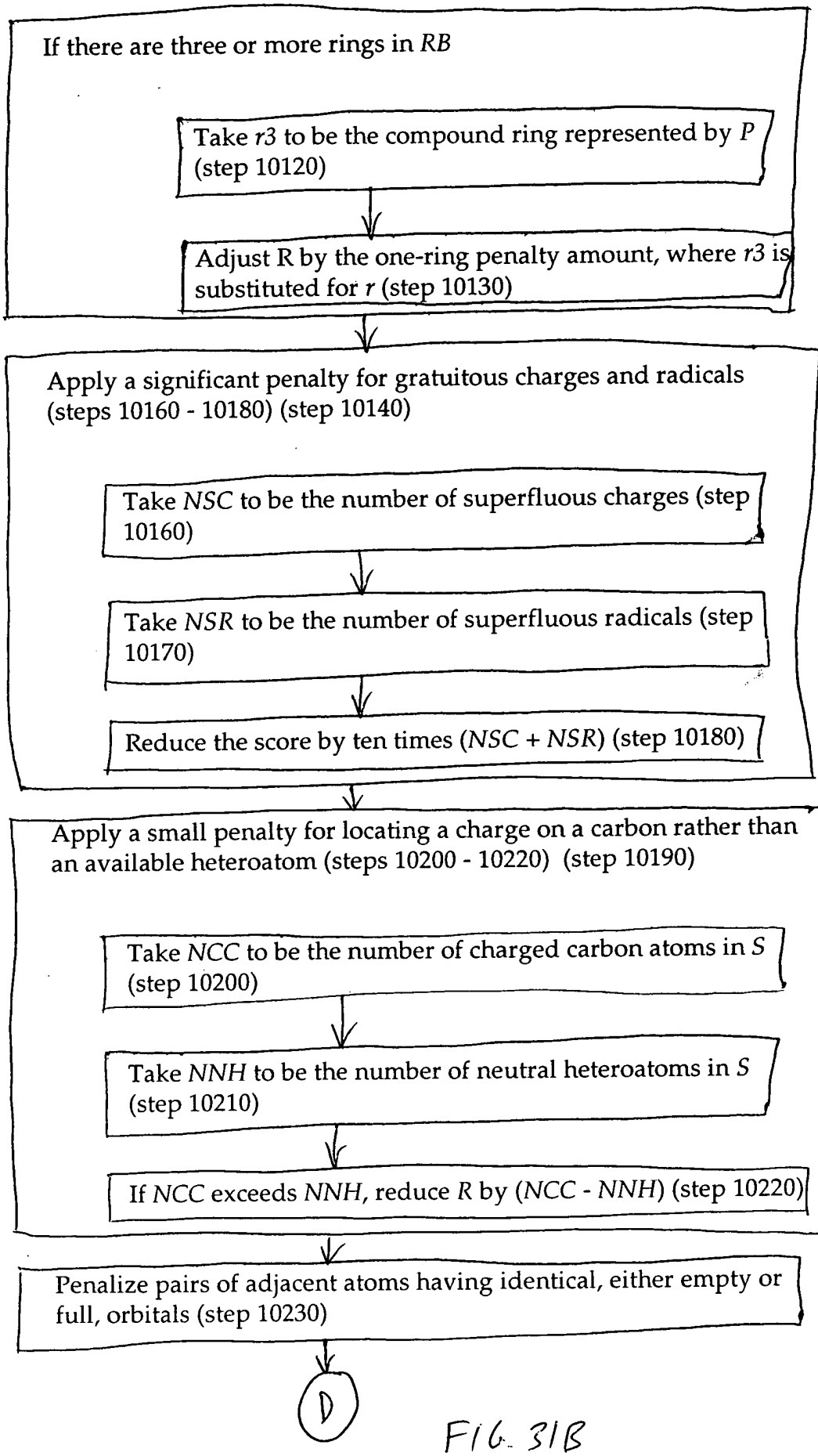

If there are three or more rings in *RB*
Take *r3* to be the compound ring represented by *P* (step 10120)
Adjust R by the one-ring penalty amount, where *r3* is substituted for *r* (step 10130)
Apply a significant penalty for gratuitous charges and radicals (steps 10160 - 10180) (step 10140)
Take *NSC* to be the number of superfluous charges (step 10160)
Take *NSR* to be the number of superfluous radicals (step 10170)
Reduce the score by ten times (*NSC* + *NSR*) (step 10180)
Apply a small penalty for locating a charge on a carbon rather than an available heteroatom (steps 10200 - 10220) (step 10190)
Take *NCC* to be the number of charged carbon atoms in *S* (step 10200)
Take *NNH* to be the number of neutral heteroatoms in *S* (step 10210)
If *NCC* exceeds *NNH*, reduce *R* by (*NCC* - *NNH*) (step 10220)
Penalize pairs of adjacent atoms having identical, either empty or full, orbitals (step 10230)
D

FIG. 31B

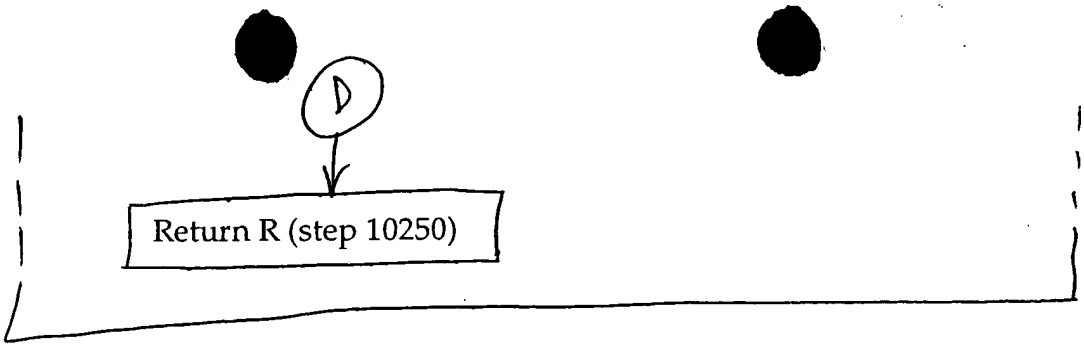


FIG. 31C